Triple Photoionization of Li and Be

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Recent intensive efforts to accurately describe the double photoionization of helium, the simplest two-electron atom, have now reached the point where almost all measurable quantities now show good agreement between experiment and several leading theoretical techniques. This process, in which the impact of one photon on the atom leads to the ionization of both electrons, is one of the cleanest systems in which electron-electron correlation plays a dominant role. Agreement between experiment and theory has been demonstrated for the total double photoionization cross section, and the differential cross sections with respect to the energy sharing and outgoing angles of both electrons.

Extensions of this work include examining the interaction between three outgoing electrons. This is most simply found in the triple photoionization of the lithium atom, in which one incoming photon results in the ionization of all three electrons of the atom. This ionization cross section was recently measured for lithium [1]. In the last few years, the time-dependent close-coupling method (TDCC) has been extended to examine this process, by treating equally the motion of all three outgoing electrons [2]. This method solves the time-dependent Schrödinger equation for all three electrons without approximation, and all electron-electron correlations are taken into account in an accurate manner. The 9-dimensional time-dependent wavefunction for the three electrons is reduced to three radial dimensions by a coupled-channel expansion over the angular momenta of the electrons. The resulting set of coupled radial differential equations is solved on a numerical lattice and propagated in time until the interaction is complete. For three electrons, the number of coupled channels which must be employed to ensure convergence can quickly become large, unlike a two-electron calculation, where perhaps 10 or 12 channels are sufficient for convergence. After this propagation, the time-dependent wavefunction for the three electrons contains *all* the scattering information about the process, including single, double, and triple photoionization probabilities. By projection onto appropriate antisymmetric spatial and spin functions, one can obtain the cross section for any of these processes. Double photoionization cross sections (where two electrons are ionized, and one electron may be left in a ground or excited state of Li^{2+}) were calculated and compared to experiment. The agreement between experiment and theory was excellent. Triple photoionization cross sections for lithium were then extracted and compared with the recent synchrotron experiments of Wehlitz et al. [1]. The cross sections are shown in Fig. 1(a); the agreement between experiment and theory is in general very good.

One can also consider similar processes in the beryllium atom. In this case, however, there are very few experiments with which to compare, as beryllium is much more toxic to work with than lithium. However, previous model calculations for the triple photoionization of beryllium indicated a much larger cross section than for lithium [3]. The time-dependent close-coupling method was therefore applied to the photoionization of beryllium, and double and triple photoionization cross sections were calculated [4]. The resulting TDCC triple photoionization cross sections, which are presented in Figure 1(b), show a much lower cross section than the previous model calculations [3]. The large difference between the two sets of calculations may be due to the neglect of the interaction between one of the outgoing electrons and the other

two electrons in the model calculations [3]. This interaction is treated fully in the time-dependent close-coupling method. It would, however, be desirable to compare these sets of calculations with experimental measurements. Such experiments, although difficult, are currently under consideration.

The time-dependent calculations discussed here make intensive use of massively parallel computing resources. Computing time at high-performance computer centers at Los Alamos, Lawrence Berkeley, and Oak Ridge national laboratories were all utilized in these calculations. We look forward to exploiting further these invaluable resources in future calculations, which include the exploration of energy sharing between all three electrons during the ionization process.

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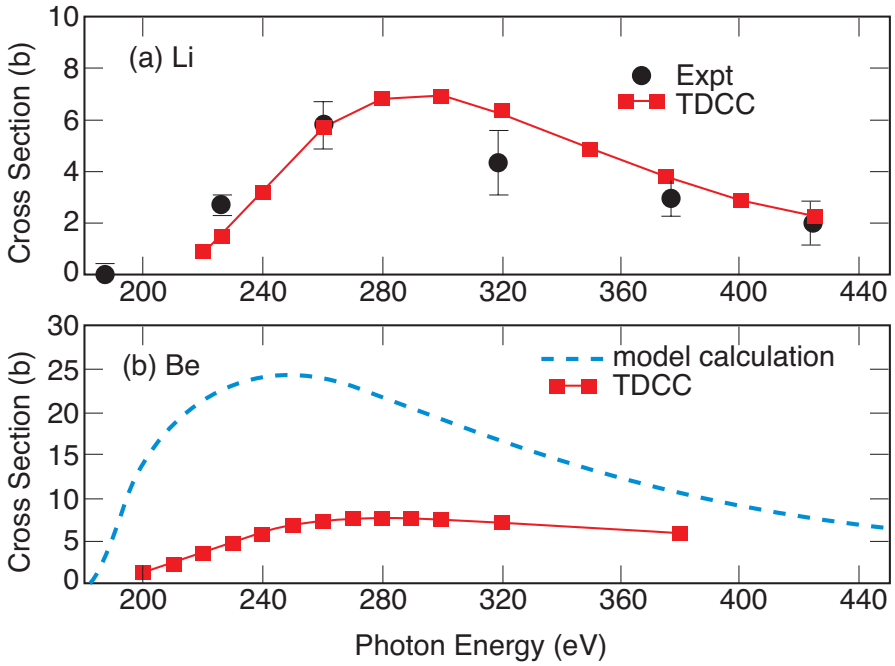

Fig. 1.
(a) Triple photoionization cross sections for lithium. (b) Triple photoionization cross sections for beryllium.